This article was published in


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Bayesian analysis of the neuromagnetic inverse problem with \( \ell^p \)-norm priors

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Received 3 December 2004; revised 3 February 2005; accepted 18 February 2005
Available online 8 April 2005

Magnetoencephalography (MEG) allows millisecond-scale non-invasive measurement of magnetic fields generated by neural currents in the brain. However, localization of the underlying current sources is ambiguous due to the so-called inverse problem. The most widely used source localization methods (i.e., minimum-norm and minimum-current estimates (MNE and MCE) and equivalent current dipole (ECD) fitting) require ad hoc determination of the cortical current distribution (\( \ell^2 \) and \( \ell^1 \)-norm priors and point-sized dipolar, respectively). In this article, we perform a Bayesian analysis of the MEG inverse problem with \( \ell^p \)-norm priors for the current sources. This way, we circumvent the arbitrary choice between \( \ell^1 \) and \( \ell^2 \)-norm prior, which is instead rendered automatically based on the data. By obtaining numerical samples from the joint posterior probability distribution of the source current parameters and model hyperparameters (such as the \( \ell^p \)-norm order \( p \)) using Markov chain Monte Carlo (MCMC) methods, we calculated the spatial inverse estimates as expectation values of the source current parameters integrated over the hyperparameters. Real MEG data and simulated (known) source currents with realistic MRI-based cortical geometry and 306-channel MEG sensor array were used. While the proposed model is sensitive to source space discretization size and computationally rather heavy, it is mathematically straightforward, thus allowing incorporation of, for instance, a priori functional magnetic resonance imaging (fMRI) information.

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Available online on ScienceDirect (www.sciencedirect.com).

Keywords: MEG inverse; Bayesian inference; \( \ell^p \)-norm; MCMC; Slice sampling

Introduction

Magnetoencephalography (MEG) allows non-invasive measurement of the magnetic fields generated by neural activity of the living brain (e.g., Baillet et al., 2001; Hämäläinen et al., 1993; Vrba and Robinson, 2001). Along with clinical applications, MEG is used in studies of basic sensory (auditory, visual, and somatosensory) processes as well as cognitive functions. Time resolution of this method is excellent (~milliseconds), but in order to locate the underlying source currents accurately on the basis of MEG data, one needs to solve the so-called electromagnetic inverse problem, which does not have a unique solution (Sarvas, 1987). Therefore, additional constraints are needed to select the most feasible estimate from the multitude of possible solutions.

A traditional approach to the MEG inverse problem is to employ the equivalent current dipole (ECD) model, which relies on the assumption that the extents of the activated areas are small enough to be adequately modeled with dipolar point-like sources. Using fully automatic or manually guided, often partly heuristic, fitting methods, the model giving best fit to the measured data is obtained. A downside is that the number and locations of the source dipoles need to be known to a certain extent (although, see Mosher et al., 1992). This is a problem especially when complex cognitive brain functions are studied.

Other widely used methods employ distributed source current estimates (e.g., Hämäläinen et al., 1993; Pascual-Marqui, 2002; Uutela et al., 1999). In the well-known minimum-norm (Dale and Sereno, 1993; Dale et al., 2000; Hämäläinen and Ilmoniemi, 1984; Hauk, 2004) and minimum-current (Uutela et al., 1999) estimates (MNE and MCE), extra information is embedded to the model as mathematical \( \ell^2 \) and \( \ell^1 \)-norm constraints on the source currents, respectively. Specifically, the least squares error function is combined with an additional penalty term consisting...
of a weighted norm of the current distribution. Unlike dipole fitting, the exact number and approximate locations of the sources do not need to be known in advance. However, the resulting estimate may be quite diffuse, especially in the case of the minimum-norm estimate and, therefore, it may be equally difficult to discern the number of distinct activated areas in practice.

In Bayesian interpretation, MNE and MCE correspond to $\ell^2$- and $\ell^1$-norm priors for the source currents with a Gaussian likelihood for the measurements (Uutela et al., 1999). The use of predefined values 1 or 2 for the $\ell^p$-norm order $p$ is somewhat arbitrary as it leads to prior-wise feasible inverse models even though any value between 1 and 2 could be used. The $\ell^2$-norm prior produces overly smooth and widely spread estimates whereas $\ell^1$-norm estimates might be too focal. The choice of $p$ is subject to uncertainty, hence $p$ should be treated as an unknown variable utilizing Bayesian inference, which has lately gained popularity in solving the electromagnetic inverse problem (e.g., Baillet and Garnero, 1997; Phillips et al., 1997; Schmidt et al., 1999). Markov chain Monte Carlo (MCMC) methods have become popular in this methodology due to rapid expansion of computing resources (e.g., Kincses et al., 2003; Schmidt et al., 1999).

In this paper, we perform a Bayesian analysis of the MEG inverse problem with $\ell^p$-norm priors, using MCMC methods and simulated source currents with a realistic MRI-based forward head model. Furthermore, we apply the model on a set of real MEG measurement data. The purpose of this study is to focus on the Bayesian interpretation of the problem, determine an optimal source space discretization size when the discretized points are assumed independent of each other, and to determine whether there is enough information in the data to clarify which $\ell^p$-norm prior should be used. We specifically hypothesize that there is no single value for $p$ that would be optimal for all cases, but instead the value depends on the grid discretization size and also on the underlying source configuration and, therefore, it should be inferred from the data rather than determined ad hoc.

Materials and methods

Simulated data were generated in order to test the performance of our model with a priori known, functionally realistic, source locations (see Fig. 1). Source space was discretized according to real anatomical MRI-based brain surface reconstruction (Dale and Sereno, 1993; Dale et al., 1999; Fischl et al., 1999) and simulated sources were then used to calculate the measurements, to which Gaussian noise was added. The spatial inverse problem was addressed with a Bayesian model utilizing numerical MCMC methods. Different grid sizes were used in order to find the optimal discretization size of the source space, and two separate source configurations were used to investigate the effect of varying signal-to-noise ratio (SNR) and underlying source extent to the spatial inverse estimate. The performance of the $\ell^1$-norm model was also tested with a real MEG data set and compared to similarly implemented $\ell^1$- and $\ell^2$-norm prior models.

Bayesian inference and Markov chain Monte Carlo methods

Bayesian inference (Gelman et al., 2003; Rowe, 2003) is a theory of probability in which both the parameters of the model and the measurements are considered as random variables. According to Bayes’ theorem (Gelman et al., 2003),

$$P(\theta | D, M) = \frac{P(D | \theta, M) \cdot P(\theta | M)}{P(D | M)}, \quad (1)$$

the posterior probability $P(\theta | D, M)$ is a product of the likelihood term $P(D | \theta, M)$ and the prior term $P(\theta | M)$, divided by the normalization factor $P(D | M)$. Above, $P(\cdot | \cdot)$ denotes a conditional probability density function, $D$ are the data, $\theta$ the model parameters, and $M$ contains all other assumptions in the model. Additional parameters in the prior term are called hyperparameters that can ultimately have higher-level prior structures leading to hierarchical models. The posterior probability distribution in Eq. (1) is generally a function of several variables and thus difficult to visualize and handle. Therefore, the distribution is often characterized by the parameters maximizing it, that is, the maximum a posteriori (MAP) estimate, or by computing suitable marginal densities. For the associated high dimensional numerical integration, Markov chain Monte Carlo methods (Gilks et al., 1996), such as the Metropolis–Hastings algorithm, are generally used (see also, Appendix B). More detailed information on Bayesian data analysis can be found in Gelman et al. (2003).

Source space

The white-gray matter boundary of cortex was reconstructed from 3-D T1-weighted high-resolution MR images (MPRAGE sequence, Siemens Sonata 1.5 T, Erlangen, Germany) using the Freesurfer software (see Dale et al., 1999; Fischl et al., 1999), with ~150,000 grid points representing each hemisphere. The resulting cortical surface geometry was overlaid over T1-weighted images for visual verification followed by transformation into MATLAB-environment, where the simulations and MCMC sampling were carried out. To parametrically optimize the size of discretization of the source space, given the assumption of statistical independence between neighboring
source locations, the number of possible source space points was reduced to ~200, ~400, ~800, ~1600, and ~3200 grid points per hemisphere. Given the widely accepted assumption that cortical currents visible to MEG are generated by synchronous post-
synaptic potentials of cortical pyramidal neurons (Dale and
Sereno, 1993; Okada et al., 1997), the orientation of the current
sources was further constrained to be perpendicular to the local
surface geometry when calculating the forward solution.

Forward model

In MEG, the Maxwell’s equations can be solved under the
quasistatic approximation assumption (Hämäläinen et al., 1993).
The solution of the forward problem gives, for one timepoint, the linear
relationship between the source currents and the measured signals

\[ \mathbf{b} = \mathbf{A}s + \mathbf{n}, \]  

where \( \mathbf{b} \) is an \( M \times 1 \) vector for measurements, \( s \) is an \( N \times 1 \) vector
for the source currents, \( \mathbf{A} \) is an \( M \times N \) gain matrix, and \( \mathbf{n} \) a
Gaussian noise vector. \( N \) is the size of the discretization of the source
space, and \( M \) is the number of measurement sensors. Each
column of \( \mathbf{A} \) gives the measured signal distribution for one dipolar
source, located on the cortical mantle and perpendicular to the cortical
surface.

For the computation of \( \mathbf{A} \), we employed the single-layer
boundary-element model (BEM), which assumes that the realistically
shaped cranial volume has a uniform electrical conductivity
and the skull is a perfect insulator. For many practical purposes,
this model is sufficient in MEG source estimation (see, e.g.,
Hämäläinen and Sarvas, 1989; Mosher et al., 1999).

For the locations of the sensors, we utilized actual data from a
measurement on the subject whose MR images were employed in
the simulation. The sensor array of the Vectorview system used
(Elekta Neuromag Oy, Helsinki, Finland) is composed of 306
sensors arranged in triplets of two planar gradiometers and a
magnetometer at 102 locations. The approximate distance between
adjacent sensor elements in the array is 35 mm and the minimum
distance of the sensor from the scalp is 17 mm.

The inverse problem

Biomagnetic inverse problem (Sarvas, 1987) stands for solving the
underlying currents in the living brain given the MEG
measurements. Mathematically, the problem involves estimating
\( s \) in Eq. (2) from samples of \( \mathbf{b} \). In this estimation task, the gain
matrix \( \mathbf{A} \) is usually assumed to be precisely known. In our model,
the number of measurements \( M = 306 \) is much smaller than the
number of points in the used grids and, therefore, the problem is
underdetermined and does not have a unique solution. Furthemore,
neighboring sensors have overlapping, non-orthogonal
sensitivity patterns (lead fields; Hämäläinen et al., 1993) and, as
a result, the number of independent equations is even less than \( M \).

The \( \ell^p \)-norm model

We present a Bayesian model consisting of a Gaussian
likelihood for the measurements and \( \ell^p \)-norm prior for the source
current parameters. In statistical terms, Eq. (2) can be written as a
linear regression model. Assuming statistically independent measure-
ments \( \mathbf{b} = [b_1, b_2, \ldots, b_M]^T \) and zero-mean \( M \)-dimensional normal
distribution for the noise, given source current parameters \( s \), the
likelihood is

\[ P(\mathbf{b} | s, \mathbf{C}) = \frac{1}{\sqrt{\det \mathbf{C}/2\pi^M}} \cdot \exp\left( -\frac{1}{2} (\mathbf{b} - \mathbf{A}s)^T \mathbf{C}^{-1} (\mathbf{b} - \mathbf{A}s) \right), \]  

where \( \mathbf{C} \) is the noise covariance matrix for the measurements. In this
study, \( \mathbf{C} \) is assumed to be known up to an unknown scaling factor
of \( \sigma_i \), so that \( \mathbf{C} = \sigma_i^2 \tilde{\mathbf{C}} \) where \( \tilde{\mathbf{C}} \) is known and diagonal. For
computational convenience, we introduce whitening of the gain
matrix, \( \mathbf{A} \), and measurements, \( \mathbf{b} \), with the known part of the noise
covariance matrix, so that

\[ \tilde{\mathbf{A}} = \tilde{\mathbf{C}}^{-1/2} \mathbf{A} \]  

and

\[ \tilde{\mathbf{b}} = \tilde{\mathbf{C}}^{-1/2} \mathbf{b}. \]  

Leaving out numerical constants, the likelihood simplifies to

\[ P(\mathbf{b} | s, \sigma_i)^2 \frac{1}{\sigma_i^{2p}} \cdot \exp\left( -\frac{1}{2\sigma_i^{2p}} (\tilde{\mathbf{b}} - \tilde{\mathbf{A}}s)^T \tilde{\mathbf{b}} - \tilde{\mathbf{A}}s \right). \]  

The scaling factor \( \sigma_i \) in the exponent function is a parameter for
compensating unknown alternations in the noise level. For
simplification, \( \sigma_i \) was assumed having a uniform prior instead of
a more conventional choice of \( 1/\sigma_i \), which would lead to uniform
prior for \( \log (\sigma_i) \). When \( M \) is large and \( \sigma_i \) close to one, then \( 1/\sigma_i^M = 1/\sigma_i^{M-1} \), and the choice of uniform prior for \( \sigma_i \) is justifiable. In the
simulation part of this study, the sampling of the posterior
distribution of \( \sigma_i \) is likely to yield values around one as the
whitening was done with a known (simulated) noise covariance
matrix. In the case of real data, \( \tilde{\mathbf{C}} \) is estimated from the
measurement data and \( \sigma_i \) would contain, for instance, information on
uncertainty of the whitening.

The \( \ell^p \)-norm for vector \( \mathbf{v} \) is

\[ \| \mathbf{v} \|_p = \left( \sum_i |v_i|^p \right)^{1/p}. \]  

In order to reduce the correlations between the formal \( \ell^p \)-norm prior
width and the source current parameters (evident in our
preliminary sampling runs), yet maintaining a continuous variable
of the norm order \( p \) for our prior, we reparametrize its structure.
First, consider a standardized normal distribution

\[ P(x) = k \cdot \exp\left( -\frac{1}{2} |x|^q \right) \]  

with \( q = 2 \).

If we let \( q \) take any values other than 2, the class of exponential
power distributions is obtained. According to Box and Tiao (1973),
(Ch. 3.2.1); with \( q = 2/(1+\delta) \) these distributions can be written as

\[ P(y | \theta, \phi, \beta) = \omega(\beta)^{-1} \exp\left( -c(\beta) \left| \frac{y - \theta}{\phi} \right|^{2/(1+\beta)} \right), -\infty < y < \infty, \]  

\[ \text{for } \theta, \phi, \text{ and } \beta. \]
where
\[
c(\beta) = \left[ \frac{\Gamma\left(\frac{3}{2} (1 + \beta)\right)}{\Gamma\left(\frac{1}{2} (1 + \beta)\right)} \right]^{1/(1+\beta)}, \quad -\infty < \beta < \infty,
\]
and
\[
\omega(\beta) = \frac{\Gamma\left(\frac{3}{2} (1 + \beta)\right)^{1/2}}{(1 + \beta)\Gamma\left(\frac{1}{2} (1 + \beta)\right)^{1/2}}, \quad \phi > 0, \quad \text{and} \quad -1 < \beta \leq 1.
\]
Parameters \( \theta \) and \( \phi \) are the mean and standard deviation of the population, respectively. In our model, Eq. (9) is written as
\[
P(s_i | \sigma_s, \beta) = \omega(\beta) \sigma_s^{-1} \exp\left(-c(\beta) \left| \frac{s_i}{\sigma_s} \right|^{2/(1+\beta)} \right), \quad \forall i = 1 \ldots N,
\]
in which the elements of vector \( s = [s_1, s_2, \ldots, s_N] \) are assumed independent, \( \theta = 0 \), and \( c(\beta) \) and \( \omega(\beta) \) are as above. \( \beta \) is a hyperparameter parameterizing the \( \ell^p \)-norm order \( p \) and \( \sigma_s \) is the variance of the source current amplitudes (prior width). In the Bayesian a priori distribution, this variance corresponds to regularization of the inverse solution and in that sense it could also be called a regularization parameter. Further on, the joint prior for the source currents is simply the product of all the independent elements
\[
P(s | \sigma_s, \beta) = \omega(\beta)^N \sigma_s^{-N} \exp\left(-c(\beta) \sum_i \left| \frac{s_i}{\sigma_s} \right|^{2/(1+\beta)} \right).
\]
The energy function corresponding to the prior is defined as a negative natural logarithm of Eq. (13)
\[
-\ln P(s | \sigma_s, \beta) = -N \ln \left( \omega(\beta) \sigma_s \right) + c(\beta) \sum_i \left( \frac{s_i}{\sigma_s} \right)^{2/(1+\beta)}.
\]
By substituting \( \beta = 0 \) and \( \beta = 1 \) to the sum expression of Eq. (14), it simplifies to
\[
\sum_i \left| \frac{s_i}{\sigma_s} \right|^2 = \frac{1}{\sigma_s^2} \sum_i |s_i|^2 = \frac{1}{\sigma_s^2} \|s\|_2^2
\]
and
\[
\sum_i \left| \frac{s_i}{\sigma_s} \right|^4 = \frac{1}{\sigma_s^4} \sum_i |s_i|^4 = \frac{1}{\sigma_s^4} \|s\|_4^4
\]
respectively.

Thus, our model imposes the \( \ell^p \)-norm (see Eq. (7)) prior for the currents so that, when \( \beta = 1 \), the model corresponds to \( \ell^1 \)-norm, and when \( \beta = 0 \), the model imposes the Euclidean norm, or \( \ell^2 \)-norm prior, for the source currents. Values \( 0 < \beta < 1 \) correspond to values of \( p \) between 2 and 1, respectively. Similarly to \( \sigma_s \) in Eq. (6), a uniform prior was also assumed for both hyperparameters \( \sigma_s \) and \( \beta \). Notice, that \( \beta \) is a hyperparameter defining the \( \ell^p \)-norm order, so that
\[
P = \frac{2}{1 + \beta}.
\]
Consequently, our choice of uniform prior for \( \beta \) will have an effect on the implicit prior of \( p \), so that the model slightly favors values of \( p \) close to 1 over the values of \( p \) close to 2. In Bayesian data analysis, this effect might be transferred to the shape of the posterior distribution of \( p \) and could be relevant in making inferences based on the analysis. With the presented \( \ell^p \)-norm model, this effect was insignificant considering our conclusions. To show this, we performed a prior sensitivity analysis for \( \beta \), which is described in a more detailed fashion in Appendix A.

Collecting the pieces of our \( \ell^p \)-norm model according to Bayes’ rule in Eq. (1) and leaving out the normalization factor which is not required for numerical considerations, the joint posterior probability distribution for the source currents \( s \), parameter \( \sigma_s \), and model hyperparameters \( \sigma_s \) and \( \beta \)
\[
P(s, \sigma_s, \beta, \beta | b) \propto P(b | s, \sigma_s) \cdot P(s | \sigma_s, \beta) \cdot P(\sigma_s) \cdot P(\beta),
\]
where model assumptions are explicitly defined in the text, hyperpriors \( P(\sigma_s) \), \( P(\sigma_s) \), and \( P(\beta) \) are assumed uniform, and \( P(b | s, \sigma_s) \) and \( P(s | \sigma_s, \beta) \) are as in Eqs. (6) and (13), respectively. In the Results and Discussion sections of the paper, we present the posterior distributions of \( p \) according to Eq. (17) and utilize only the parameter \( p \) to facilitate the reading.

Simulated data sets

We utilized four functionally relevant source locations in data simulations: the left motor cortex (S1), left dorsolateral prefrontal cortex (S2), right posterior superior temporal sulcus (S3), and right primary auditory cortex (S4). With each location, at least three source extents were used. The first source extent contained only a single active source space point (0-neighborhood). The other types contained 1- and 2-neighborhoods of the one center point along the original source space grid. On average, these correspond to point-sized, ~0.2 cm², and ~0.7 cm² physical sizes on the white-gray matter boundary. In this paper, the source extent is denoted with subindex (e.g., S1o). The anatomical locations and sources are shown on the inflated white-gray matter boundary in Fig. 1. Mainly, we simulated single sources, but also combinations of sources were studied so that the total number of different source configurations that were used to determine the optimal grid discretization size was 21. To investigate the effect of the extent of the underlying source configuration, two sources (S1 and S4) were additionally analyzed with 4- and 8-neighborhoods (~3 cm² and ~15 cm², respectively). The source current amplitude was set to be 80 nAm for the whole source regardless of its extent. For the combinatorial sources S5 (S1 and S2 active together), the source current amplitudes were 80 nAm for both or alternatively 80 nAm for one and 40 nAm for the other.

Data were generated by using the forward model in Eq. (2) to create the fields for one timepoint. Maximum amplitudes of the resulting magnetic fields and magnetic field gradients were realistic, approximately 200–400 fT for magnetometers and 50–200 fT/cm for gradiometers. The gain matrix \( A \) used in the forward computation included 306 rows and approximately 32,000 columns. This way, the original source space grid size contained ~16,000 points per hemisphere and consequently, as the solution grid sizes were all significantly smaller, the most obvious type of inverse crime was avoided. The term inverse crime is used to describe all those elements that are fixed in the data generating model and later presumed known in the solution part. Naturally, in simulation studies such modeling flaws might lead to improved and too optimistic results, but also to overfitting and spurious models which would likely fail in real data scenarios.
Random zero-mean Gaussian noise was added to the simulated measurement vector $\mathbf{b}$, so that the mean signal-to-noise ratio described by

$$\text{SNR} = \frac{\mathbf{b}^T \mathbf{b}}{M \sigma_n^2}$$

was 15 for magnetometers and about 60 for gradiometers. $M$ is the number of sensors and $\sigma_n$ is the standard deviation of the corresponding sensor noise. The measurement noise was assumed equal separately within the three sets of different sensors (i.e., two sets of gradiometers, one set of magnetometers). In most cases, SNR was set to be rather good, because we were mainly interested whether there is information in the data to determine the norm order $p$. The effect of SNR to the model was examined with two sources $S_1$ and $S_4$, so that the mean SNR for gradiometer measurements was approximately 5, 15, 30, 60, and 90 (1.25, 3.75, 7.5, 15, and 22.5 for magnetometers). After adding the noise, the simulated data were whitened according to Eq. (5).

Real MEG data

The real MEG data set contained evoked fields of a self-paced index finger lifting experiment of a one right-handed male, aged 27. There were two conditions: the subject lifted his (A) right and (B) left index finger. Electro-oculogram (EOG) artefact rejection threshold (peak-to-peak) was set to 150 $\mu$V, so that 111 accepted trials were averaged in the first condition and 113 in the second one. The measured data vector $\mathbf{b}$ was taken at a latency of 20 ms from the onset of finger movement in both conditions. The known part of the noise covariance matrix $\mathbf{C}$ (see Eq. (5)) was estimated as a variance of each sensor from a 2-min fragment of filtered measurement data acquired when the subject was sitting in the shielded room under the MEG device doing nothing prior to the actual experiment. To reflect the decrease of noise due to averaging, $\mathbf{C}$ was scaled by dividing it by the number of trials averaged separately for both conditions. A Hamming window based digital filter was used to remove noise from the averaged evoked fields and the fragment of data from which $\mathbf{C}$ was estimated. The passband edge frequencies were [2 18] Hz and stopband edge frequencies [0.5 20] Hz. The estimated mean signal-to-noise ratio for the utilized data was approximately 6/0.1 for condition A gradiometer/magnetometer measurements and 8/0.1 for condition B. However, the sensors that mostly contained the signal (i.e., the best SNR) had a fairly good SNR of about 40–70 for gradiometers and 1–2 for magnetometers.

Sampling procedure and inverse estimation

All parameters of the model, including source currents $\mathbf{s}$, hyperparameter $\beta$, likelihood standard deviation $\sigma_l$, and prior width $\sigma_c$, were considered as random variables and their distributions were obtained utilizing an MCMC method called slice sampling. Samples were drawn from the joint posterior distribution of the currents and model parameters (Eq. (18)) using modern Linux-workstations (Pentium III/4, 1–3.2 GHz processor, 1024–4096 MB of RAM). Slice sampling is often more efficient than simple Metropolis updates as it adaptively chooses the magnitude of the changes made. Convergence diagnostics and time series analysis, such as potential scale reduction factor (PSRF), were used to verify that the convergence of the sampler was plausible (Robert and Casella, 2004). For more information on utilized sampling method and convergence diagnostics, see Appendix B.

The inverse estimates were calculated as posterior expectation values of the currents integrated over the hyperparameters $\beta$, $\sigma_c$, and $\sigma_l$. This was done for all the simulated sources using the $\ell^q$-norm prior model. For visualization purposes, the estimates on each grid size were thresholded by setting to zero the current amplitude of all the source points whose absolute amplitude value did not exceed 20% of the peak value of that particular estimate. In most cases, the solution estimates were also interpolated on the original cortical mantle (~16,000), so that the visual comparison with the simulated solutions would be easier.

Model choice

In addition to the visual examination of the quality of the solutions, the model goodness was estimated with a method based on posterior predictive sampling. Gelfand and Ghosh (1998) propose a minimum posterior predictive loss approach in which the criterion, whose minimum defines the optimal model, comprises of a goodness-of-fit term $G_m$ and a penalty term $P_m$, where $m$ denotes the model. In our study, the term $G_m$ was calculated as a sum of squared error of the model predicted measurements averaged over 21 different sources that were used in the analysis, and $P_m$ was determined by the sum of predictive variances of the measurements. The posterior distribution of the measurements was attained by computing it using the forward model in Eq. (2) with the source current samples. In this particular case, the posterior predictive sampling is easy to do as we already have a large amount of Monte Carlo samples obtained from the posterior distribution. The minimum posterior predictive loss criterion for model $m$, $D_m = G_m + P_m$ (Gelfand and Ghosh, 1998), was calculated as an average over all the sources analyzed in this study, and thus considering the grid size as a variable altering the model structure. Furthermore, our $\ell^q$-norm model was compared with similar $\ell^1$- and $\ell^2$-norm prior models by analyzing simulated data sets shown in Fig. 1. These models were realized as special cases of the $\ell^p$-norm model by setting the hyperparameter $\beta$ to 1 and 0, respectively. Based on the obtained posterior distributions, we also performed model choice using the minimum posterior predictive loss approach.

Results

An MCMC chain was produced for each of the simulated sources and for each of the grid sizes separately. For the smaller grid sizes (~200, ~400, and ~800 points per hemisphere), the time required to draw one sample (i.e., one set of source current parameters and hyperparameters) from the joint posterior distribution was in the order of 1–4 s. At least 10,000 samples were drawn for each of these chains. For the chains of the larger grid sizes (~1600 and ~3200 per hemisphere), the time required for one sample was about 10–25 s. Despite the time-consuming computer runs, at least 3000 samples were drawn for these chains.

The convergence of the sampler appeared to be plausible by the potential scale reduction factor (see Appendix B.2), which was estimated either for the different segments of one chain or from several chains of the same source with different initial conditions. The chains seemed to converge also based on visual inspection of the obtained samples. Time series analysis revealed that autocorrelation times of the samples were in general quite long. For some source current parameters and hyperparameters, the autocorrelation
time was in the order of several hundreds or even over one thousand samples. This means that from a chain of 10,000 samples we get effectively only ~50 independent samples or even less. Inverse estimates were obtained from these independent samples by implicitly integrating the posterior of source current parameters over the hyperparameters and computing the expectation value for $s$. Low number of independent samples increases the Monte Carlo error of this estimate, but 10–50 is enough for a reasonable one.

Inverse estimates for simulated sources $S_{10}$, $S_{21}$, and $S_{41}$ are shown with the original sources in Fig. 2. The utilized grid sizes for sampling these inverse estimates were ~800 ($S_{10}$) and ~1600 ($S_{21}$ and $S_{41}$) per hemisphere. $S_{10}$ represents a fairly superficial and focal source on the left motor cortex whereas $S_{41}$ is a deeper source in the right auditory cortex. These solutions are representatives of the best and worst case estimates obtained with our model for smaller source extents. Quite often, the estimate produced by the $\ell^p$-norm model is located in the neighboring sulcus and oriented almost identically as the original source. For example, even though the peak value of the solution estimate in Fig. 2A is not on the same sulcus and over 2 cm away from the original source along the cortical surface (~1 cm in 3-D), the estimate fits the original data well (within the noise limits) as can be seen in Fig. 3B. This is because the small amount of current in the correct gyrus is compensated with a larger amount in the neighboring gyrus (see Fig. 3A). As a result, these activations produce similar fields to what the original simulated source does. As MEG is fairly insensitive to small locational discrepancies when measured from a distance (outside the scalp), this type of solutions when computed through the forward model gives rise to excellent fits with the original measurement data. The $\ell^p$-norm model estimate in Fig. 2B looks relatively good, and the deeper source in Fig. 2C is spread on the source points closer to surface.

The $\ell^p$-norm inverse estimates for simulated sources in Fig. 1 are shown in series of Figs. 4–6. It is seen that with smaller grid sizes (less than ~1600 points per hemisphere; see Fig. 4) only the major cortical structures are visible and the localization accuracy is limited.
by the grid discretization size. With the larger discretization sizes (more than ~1600 points per hemisphere; see Figs. 5 and 6), the estimates of the 0-neighborhood sources are spread when the original source is a deep or a combinatorial source, whereas especially with the combinatorial sources the larger source extents (2-neighborhoods) are more locally localized. However, with a wider superficial source (e.g., S12), the estimate gets more diffuse. With the grid size of ~1600 (Fig. 5), the estimates of the $\ell^p$-norm model look rather satisfactory with respect to the model assumptions.

Histograms of the posterior distribution samples of model parameters $\sigma_c$, $\sigma_l$, and the $\ell^p$-norm order $p$ for some of the abovementioned simulations are visualized in Fig. 7. It is clearly seen that $p$ (upmost row in each subfigure in Fig. 7) is dependent of the source configuration as well as the grid size. For instance, the distributions of $p$ for grid size ~1600 per hemisphere with sources S10 and S30 are different. The distribution shapes also vary through the same source configuration depending on the grid size. For $p$, with source S3 and grid size ~3200, the most probable value of the posterior distribution is clearly different from the most probable value with smaller grid sizes. In most cases, the $\ell^p$-norm model seems to lean towards the $\ell^1$-norm model ($p = 1$), but this is not the case, for instance, with the abovementioned source and grid size for which the most probable value of $p$ is somewhere between 1 and 2. The tendency of the $\ell^p$-norm order $p$ to favor values close to 1 is not a manifestation of the implicit prior for $p$, but as our prior sensitivity analysis reveal, it is an effect that is caused inherently by the data (see Appendix A). In all situations, the expectation value of $\sigma_l$ is close to one, as was hypothesized. Notably, the distribution of the regularization parameter, or prior width $\sigma_c$, tends to be extremely narrow with larger grid sizes. This suggests that with a dense grid, manual choice of the regularization parameter is more difficult.

The results of analyzing sources S1 and S4 with a wider range of source extents and grid size ~1600 are shown in Figs. 8 and 9. With source S1 on the left motor cortex (Fig. 8), the inverse estimate seems to spread as the source extent gets larger. Especially with the widest extent (S18), the inverse estimate is spread throughout the cortex and does not look acceptable. Notably, the posterior distribution of $p$ is similar with all the source extents even though with the larger extents the distribution seems to be somewhat wider. The distribution of prior width $\sigma_c$ is slightly peaked with 4- and 8-neighborhoods. Source S4 on the right auditory cortex (Fig. 9) seems to be equally well localized regardless of the underlying source extent. The hyperparameter posterior distributions look similar with different source extents except for the distribution of $p$, which is not so strongly peaked towards $p = 1$ as was the case with source S1 in Fig. 8.

Sources S1 and S4 were analyzed with a range of different signal-to-noise ratios. The corresponding inverse estimates are shown in Fig. 10 and labeled with gradiometer mean SNR, respectively. The utilized grid size was ~1600 per hemisphere.

Figures 5 and 6. Inverse estimates calculated from the analysis of the $\ell^p$-norm model with grid size ~1600 points per hemisphere.
Fig. 7. Histograms of the samples of the posterior distributions of the hyperparameters $p$, $\sigma_c$, and $\sigma_I$ from the simulations of the sources S10, S30, S11, and S31 for different grid discretization sizes per hemisphere.

Fig. 8. The simulated source S1 with 0-, 1-, 2-, 4-, and 8-neighborhoods is plotted on the white-gray matter boundary on the top row. The $\ell^p$-norm estimates with grid discretization size ~1600 are shown on the second row. For the corresponding estimates, the posterior distributions of the model parameters $p$, $\sigma_c$, and $\sigma_I$ are shown below.
parameters as well as inverse estimate fits to measured data for both conditions are also presented in Fig. 12. With real data, the model seems to favor values of $p$ closer to 1 than 2. The estimates produce a good fit with the data in both conditions even though the magnetometer measurements had in general quite poor SNR.

We also analyzed the data with the models where $p$ equals 1 and 2, corresponding to $\ell^1$- and $\ell^2$-norm prior models. In Fig. 13, the obtained inverse estimates for simulated source S11 are shown. Notably, the $\ell^2$-norm estimate is more diffuse on fairly large areas at the parietal cortices whereas $\ell^1$- and $\ell^p$-norm estimates are spatially of smaller extent. Typically, the inverse estimates obtained with $\ell^p$- and $\ell^1$-norm models were more focal and visually similar to each other whereas the $\ell^2$-norm model estimates were more extensive. The source current parameter expectation values were smaller in the $\ell^2$-norm estimates as this prior tends to impose little current on number of source space points rather than large amount of current on very few points. The standard deviations of the posterior distribution Monte Carlo samples for those estimated source current points whose absolute amplitude exceed 20% of the maximum absolute amplitude of the estimate are plotted as one sigma error bars to the figure for each estimate, respectively. In many cases of our simulations, these Monte Carlo variances of the source current parameters were considerable. However, the posterior expectation value is still a credible indicator of which of the parameters were non-zero, because even with a small number of independent samples, the uncertainty of this estimate is relatively small.

For the model choice, the resulting posterior predictive loss criterion (Gelfand and Ghosh, 1998) as a function of grid discretization size is shown in Fig. 14A and the comparison between the $\ell^p$-, $\ell^1$-, and $\ell^2$-norm priors in Fig. 14B. According to this approach, the optimal grid discretization size for our $\ell^p$-norm model is around 1000–2000 points per hemisphere (see the minimum of curve in Fig. 14A). The visual examination of the $\ell^p$-norm estimates using grid size of ~1600 points per hemisphere (see Fig. 5) yielded similar findings. For the comparison of different norms, the results obtained with the posterior predictive

![Fig. 9. The simulated source S4 with 0-, 1-, 2-, 4-, and 8-neighborhoods is plotted on the white-gray matter boundary on the top row. The $\ell^p$-norm estimates with grid discretization size ~1600 are shown on the second row. For the corresponding estimates, the posterior distributions of the model parameters $p$, $\sigma_c$, and $\sigma_l$ are shown below.](image)

![Fig. 10. The inverse estimates of sources S12 and S41 with varying signal-to-noise ratios. The SNR label denotes the mean signal-to-noise ratio of the gradiometer measurements of the corresponding source. The original simulated sources S12 and S41 can be seen in Figs. 1 and 2. The utilized grid size in the analysis was ~1600 per hemisphere.](image)
loss approach were indecisive even though the $\ell^2$- and $\ell^1$-norm estimates were visually more satisfying than the $\ell^2$-norm estimates.

**Discussion**

We studied a Bayesian MEG inverse model with $\ell^p$-norm priors for the source currents. This type of model has not been implemented before, even though similar ideas considering different values of $p$ have been suggested (e.g., Beucker and Schlitt, 1996; Bücker et al., 2001; Matsuura and Okabe, 1995; Uutela et al., 1999). Using Bayesian methodology, the full joint posterior distribution of the parameters and hyperparameters of the model, such as the $\ell^p$-norm order $p$ and prior width $\sigma_c$, can be obtained. From the posterior distribution, one is able to compute quantiles, moments, and other summaries of interest as needed. The purpose of our study was to find an optimal source grid spacing for the $\ell^p$-norm model, to show that there is no universal correct value for the norm order $p$. It was also demonstrated that this effect observed in the posterior distribution of $p$ was not due to the implicit prior for slightly favoring values of $p$ closer to 1 over 2 (see Appendix A). Therefore, a good way would be to let the source current prior (i.e., the value of $p$ when utilizing $\ell^p$-norms) be inferred from the data, instead of determining it ad hoc, as long as the basic properties of the prior are defined to be realistic.

An MCMC sampling scheme was utilized as we were interested in the posterior distributions of all the parameters and did not want to make any uncontrolled analytical approximations that might have some unexpected qualities. With MCMC, the posterior expectation values can be computed reliably as the error due to Monte Carlo estimation is quite small even with small number of independent samples. In addition, one is able to investigate the whole posterior distribution of the solutions and is not limited to conclusions based only on the MAP estimate. As demonstrated by Schmidt et al. (1999), the use of the most likely solution is not necessarily representative for constructing robust and reliable inferences from the data. In our study in Fig. 11 (S41, SNR = 5), it was seen that the maximum of the marginal posterior for $p$ is not where the most probability mass lies and the distribution might even be multimodal. Similar situations may occur also in the

![Fig. 11. Histograms of the samples of the posterior distributions of the model hyperparameters $p$, $\sigma_c$, and $\sigma_l$ from the simulations of the sources S12 and S41 with varying SNR. The utilized grid size in the analysis was ~1600 per hemisphere.](image-url)
posterior distribution of the parameters of interest (source currents). In that case, if the posterior is multimodal, the importance of making inferences from the whole posterior rather than MAP estimate becomes absolutely crucial.

Beucker and Schlitt (1996) showed that the density of source locations has an effect on the norm order $p$. Our results indicate that a dense discretization seems to favor values of $p$ closer to 2. The optimal discretization size for our model was ~1500 points per hemisphere. If number of sources is decreased to 200–400 points per hemisphere, the accuracy of the estimates is not good and the model does not fit the data well, because the grid is too sparse and only major cortical structures are visible. As the discretization size increases, the goodness-of-fit improves, but with really dense grids the proposed $\ell^p$-norm model becomes unacceptably heavy to compute, and at the same time the model prior assumption of independent source currents is severely violated.

Fig. 12. Results of the analysis of the real MEG finger lifting data with the $\ell^p$-norm model (grid size ~1600). The conditions were (A) right and (B) left index finger lifting. For both conditions, the predicted data are plotted (red line) on top of measurement data (blue dots) with one sigma error bars separately for each gradiometer and magnetometer sensors. Histograms of the posterior samples of $p$, $\sigma_c$, and $\sigma_l$ are also shown to visualize the shapes of the marginal posterior distributions.

Fig. 13. Simulated source S11 and its corresponding inverse estimate with the $\ell^p$, $\ell^1$, and $\ell^2$-norm models using grid size ~800. The solution estimates are interpolated on the original cortical mantle (~16,000) for visualization purposes on the top row and shown as vector values with Monte Carlo sampling standard deviation error bars (both hemispheres) in the bottom row. Only the values that are at least 20% of the estimate peak value (dotted red lines) are plotted on the inflated brain and only corresponding error bars are shown. Note that the current amplitude values obtained with the $\ell^2$-norm model are smaller and the estimate is the most diffuse out of these three.
One way to ease the computational load would be to decrease the number of parameters by parametrizing the sources. For example, Schmidt et al. (1999) employed regional source model, which was characterized by three parameters comprising of number, location, and extent of the active regions. This way, they decreased the number of parameters sampled from several thousands to only three (per activity region). In this case, one introduces some spatial dependency to the model as the points inside the active regions are assumed to correlate strongly. The assumption of uncorrelated source space points seems justifiable in early sensory responses while in complex cognitive tasks one may expect correlations not only between neighboring points but between remote cortical regions as well. However, taking this into account in the inverse model is not necessarily straightforward due to the absence of data on the exact nature of the correlations.

A conceivable way to take into account the putative dependencies between source space points would be to introduce spatial priors. Furthermore, with the current $\ell^p$-norm model, the grid discretization size cannot be increased unless spatial priors are used. As the most feasible spatial priors are neither simple nor intuitive, there exists some unclarity of which kind to use. Phillips et al. (2002) suggest that the combination of functional and anatomical constraints might provide a way for introducing spatial priors to the model and at the same time for reducing the dimensionality of the MEG inverse problem. With real data scenarios, one has to remember that some sources are not visible for MEG and therefore the use of spatial priors becomes even more important if additional information is not available from elsewhere. The implementation and testing of such justifiable spatial priors is left for subsequent studies.

Converging evidence from other imaging modalities, such as functional magnetic resonance imaging (fMRI) and electroencephalography (EEG), can be introduced to the current $\ell^p$-norm model if the utilized experimental setup is suitable for collecting data with various methods. The combination of adjacent imaging methods (Dale et al., 2000; Liu et al., 2002), MEG with fMRI in particular (Ahlfors and Simpson, 2004; Dale et al., 2000; Schulz et al., 2004), is going to be an invaluable tool in brain research in the future. Even if the coupling between fMRI BOLD signal and EEG/MEG response is not well understood, clear evidence exists on how these two fundamentally different signals are related (Kim et al., 2004; Logothetis et al., 2001). In comparison, the combined use of MEG and EEG is relatively straightforward as both of these methods detect the neural electric currents. Since EEG provides information about the radial currents in addition to the tangential ones detected by MEG, it is conceivable that the combination will provide a more comprehensive estimate of the underlying neural events.

However, as Liu et al. (2002) and Phillips et al. (1997) suggest, the combination of EEG and MEG might not improve the results much. Furthermore, with EEG inverse modeling, there exists the problem of creating a realistic forward model for EEG as in that case the electric conductivities of the scalp, the skull, and the brain tissue and the shapes of the corresponding compartments need to be known more precisely (Ollikainen et al., 1999). In contrast, an a priori bias towards fMRI information is straightforward to add to the current model per se. In addition, depth normalization can be included to reduce the location bias of the estimates (Köhler et al., 1996) and, with the cost of computational burden, the use of temporal dynamics in the model might prove to be useful especially for empirical investigations.

Our preliminary analysis with real MEG data were promising. The results are in line with similar MEG studies in the field (see, e.g. Alary et al., 2002). However, the application of the model with more complex real data (e.g., cognitive tasks and audiovisual studies) still requires work and implementation of some of the abovementioned methods such as spatial priors and temporal dynamics. As of now, the $\ell^2$-norm model is a spatial only MEG source localization method.

The quality of MEG inverse estimates in general is not trivial to evaluate even though in simulation studies the original sources are known. In addition to the visual quality of the solution estimates, one can, for example, easily approximate the physical distance between the solution peaks and original sources both along the cortical surface and in 3-D and use this as a quantitative error. But the question arises how to penalize false activations, for instance, in situations where the solutions are spread over the cortex, and how to penalize the goodness of the solution if the estimate is located in the wrong gyrus yet being highly probable (see Fig. 3). In the analysis of real data, particularly, when the original sources are not known, different methods are needed. One way is to look at all the solutions and compare different models with each other instead of single estimates and their accuracy. One such method is the posterior predictive loss approach (Gelfand and Ghosh, 1998), which we used, along with visual examination, to determine the optimal discretization of the source space for our $\ell^p$-norm model.

On top of being able to evaluate the whole posterior distribution of the parameters and hyperparameters, which conceal information of the model behavior and inverse estimates, a substantial benefit of our model is that it is very simple and therefore additional (prior)
information is easy to attach. Virtually no user expertise is required after the model is compiled and the method can be used almost without any manual interaction or tuning, which is not the case with ECD fitting. This feature is more or less fundamental with many Bayesian models. Naturally, an experienced user can achieve excellent results with methods that require more interaction, but a problem arises if one’s goal is to study cognitive processes about which very little is known in advance. In those cases, a model that does not require tuning would be most convenient to use. The estimates obtained with our $\ell^p$-norm model can also be used as a starting point for seeds for other source localization methods. This is practical when little is known of the sources under investigation.

(Ch. 1.8): Suppose that effects and extra terms it has on the outcome. Gelman et al. (2003), metrization to another, one needs to carefully consider what kind of

Appendix A. Prior sensitivity analysis for

Wihuri Foundation. Authors would like to thank anonymous Health (RO1-HD40712), The MIND Institute, and Jenny and Antti

Acknowledgments

This research was supported in part by Academy of Finland (projects: 200521, 202871, 206368), Instrumentarium Science Foundation, Finnish Cultural Foundation, National Institutes of Health (RO1-HD40712), The MIND Institute, and Jenny and Antti Wihuri Foundation. Authors would like to thank anonymous reviewers for helpful remarks and Mr. Antti Yli-Krekola for a helping hand with the preprocessing of MR-images.

Appendix A. Prior sensitivity analysis for $\beta$

When transforming probability distributions from one parametrization to another, one needs to carefully consider what kind of effects and extra terms it has on the outcome. Gelman et al. (2003), (Ch. 1.8): Suppose that $P_u(u)$ is the density of vector $u$ and we want to transform to $v = f(u)$. If $P_u$ is continuous and $v = f(u)$ is a one-to-one transformation, then the joint density of $v$

\[ P_v(v) = |J| \cdot P_u(f^{-1}(v)), \]

where $|J|$ is the determinant of the Jacobian of the transformation $u = f^{-1}(v)$. The Jacobian $J$ is a square matrix of partial derivatives, with the entry $(i,j)$ equal to $\partial u_i / \partial v_j$.

A.1. Uniform prior for $\beta$

If we want to transform to using $p$ with the utilized parametrization (Box and Tiao, 1973) of our $\ell^p$-norm model having uniform prior probability density for $\beta$ and $f(\beta)$ being Eq. (17), we get by rearranging Eq. (17)

\[ f^{-1}(p) = \frac{2}{p} - 1, \quad 0 \leq \beta \leq 1, \quad \text{and} \quad 1 \leq p \leq 2. \]  

The Jacobian for $f^{-1}(p)$ is simply the derivative

\[ \frac{d\beta}{dp} = \frac{d}{dp} \left( \frac{2}{p} - 1 \right) = -\frac{2}{p^2}, \]  

and the probability density of $p$

\[ P(p) = \left| -\frac{2}{p^2} \right| \cdot P(\beta), \quad 0 \leq \beta \leq 1, \quad \text{and} \quad 1 \leq p \leq 2. \]  

Thus, the implicit prior for $p$ in our $\ell^p$-norm model with uniform prior for $\beta$ only slightly favors values of $p$ close to 1 over values of $p$ close to 2 as the determinants of the Jacobian at the endpoints of $p$ are 2 and 0.5, respectively.

A.2. Uniform prior for $p$

Consider another possibility for our model by choosing a uniform prior probability density for $p$. With the parametrization used, when transforming to using $\beta$, we get the Jacobian as

\[ \frac{dp}{d\beta} = \frac{d}{d\beta} \left( \frac{2}{1 + \beta} \right) = -\frac{2}{(1 + \beta)^2}, \]  

and the probability density of $\beta$

\[ P(\beta) = \left| -\frac{2}{1 + \beta} \right| \cdot P(p), \quad 1 \leq p \leq 2, \quad \text{and} \quad 0 \leq \beta \leq 1. \]  

Now the implicit prior for $\beta$ will slightly favor values of $\beta$ close to 0 over values of $\beta$ close to 1 as the determinants of the Jacobian at the endpoints of $\beta$ are 2 and 0.5, respectively. This converts to favoring values of $p$ close to 2 over values of $p$ close to 1, which is opposite to the case of uniform prior for $\beta$.

A.3. Sensitivity analysis

In addition to the analysis done with our selection of uniform prior for $\beta$, we analyzed some of the simulated sources ($S_{1D,2}$ and $S_{3D,3}$ with grid sizes ~800, ~1600, and ~3200) with the choice of uniform prior for $p$. This was done in order to validate that the effects observed in the posterior distribution of $p$ were, in fact, caused by the data and not by the implicit shape of the utilized prior distribution. In Fig. 15, one can see the envelope curves of the posterior distributions of $p$ for the $\ell^2$-norm model with a uniform prior for $\beta$ (blue curve) and uniform prior for $p$ (red curve). The shapes of the (implicit) prior distributions of $p$ are shown with dotted curves, respectively. As the posterior shapes in general are significantly different from the prior shapes, it is clear that posterior distributions yield values closer to $p = 1$ regardless of which prior was used. The slight inconsistency with source $S_{3D}$ (grid size ~3200, red curve) is most likely due to the fact that the corresponding chain with the uniform prior for $p$ did not have enough independent samples.

Appendix B. Sampling method and diagnostics

B.1. Slice sampling

In Bayesian data analysis (Gelman et al., 2003), applications of Markov chain Monte Carlo sampling often involve retrieving samples from the joint posterior distribution of the parameters and hyperparameters of the model. In Metropolis–Hastings scheme,
badly selected scale of the proposal distribution leads to high rejection rate or inefficient random walk. Slice sampling (Neal, 2003) relies on the principle that one can sample uniformly under the curve of some known probability density function $P(d)$. With slice sampling, unlike in Gibbs sampling (Gilks et al., 1996), the conditional distributions of standard form do not need to be known, and with multimodal distributions slice sampling is often more efficient than simple Metropolis–Hastings algorithm in making jumps from one mode to another. Slice sampling adapts to the local properties of the target distribution and it requires very little tuning. With multidimensional distributions, each variable can be updated in turn.

A converging Markov chain towards the target distribution can be obtained by sampling uniformly by turns in vertical direction under the curve and horizontally from a slice defined by this vertical position. Let the variable to be updated be $x$ and $f(x)$ the function proportional to the probability density of $x$. The idea for producing a chain for $x$ is to replace the current value $x_{\text{old}}$ with a new value $x_{\text{new}}$. Draw a real value of $y$ from $0 < y < f(x_{\text{old}})$ which defines a horizontal slice $S = \{x: y < f(x)\}$. Find an interval $I$ around $x_{\text{old}}$ that contains much or all of the slice $S$. Now, draw $x_{\text{new}}$ uniformly from the part of the slice within interval $I$ and repeat the procedure. There are several different schemes for finding the interval $I$ that are well covered in the work by Neal (2003). In fact, the interval can be chosen in any way as long as the resulting Markov chain remains invariant.

For computational purposes, in order to avoid possible problems with floating-point underflow, an energy function of $g(x) = -\ln(f(x))$ is often calculated instead of $f(x)$ itself. With this particular case, a variable $z = \ln(y) = -g(x_{\text{old}}) - e$ can be calculated to define the slice $S = \{x: z < -g(x)\}$. Variable $e$ is exponentially distributed with mean one. Furthermore, for our simulations, as the sampling was done one variable (source current parameters $s = [s_1, s_2, \ldots, s_N]$, $\beta$, $\sigma_e$, and $\sigma_i$) at a time, we optimized the performance of the sampler by updating only the change caused by this particular variable to the value of the energy function of the joint posterior distribution rather than computing it completely every time each variable was updated.

### B.2. Convergence diagnostics

There are two types of difficulties with iterative simulations such as MCMC simulations. The simulations might not have been proceeded long enough so that the resulting samples are not yet representative of the target distribution. The early iterations are also influenced by the starting point rather than the target distribution. After a plausible convergence is reached, the chain has forgot its starting point and produces representative values of the target
distribution. The early iterations are removed from the beginning of the chain. The other problem lies in the correlation within the converging chain. In general, it is better to start several chains with different starting points especially if the autocorrelation time of the chain is long. This way, when the chains have converged, the number of independent samples is greater than with one long chain. However, all the converged samples can still be used as the order in which they were drawn is ignored when performing inferences based on their distributions.

A chain can be assumed to have converged when two chains originating from different starting points can no longer be differentiated from each other. One method in monitoring the convergence is to compare the variances between different chains or different segments of one chain and estimate a factor by which the scale of the current distribution might be reduced if the sampling was continued to infinity. The procedure of calculating this potential scale reduction factor (PSRF) is described in Gelman et al. (2003), (Ch. 11.6).

References


